2-Butyn-1-yl chloroformate

Inchi: InChI=1S/C5H5ClO2/c1-2-3-4-8-5(6)7/h4H2,1H3
InchiKey: MFKKPMUEGDJJSL-UHFFFAOYSA-N
Formula: C5H5ClO2
SMILES: CC#CCOC(=O)Cl
Mol. weight [g/mol]: 132.54
CAS: 202591-85-3

Physical Properties

Property code	Value	Unit	Source
gf	-51.83	kJ/mol	Joback Method
hf	-134.77	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.385		Crippen Method
mcvol	92.390	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
tb	436.52	K	Joback Method
tc	649.34	K	Joback Method
tf	354.29	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.23	J/mol×K	436.52	Joback Method
cpg	163.79	J/mol×K	471.99	Joback Method
cpg	170.14	J/mol×K	507.46	Joback Method
cpg	176.27	J/mol×K	542.93	Joback Method
cpg	182.16	J/mol×K	578.40	Joback Method
cpg	187.82	J/mol×K	613.87	Joback Method
cpg	193.23	J/mol×K	649.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C202591853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume